Subtle interface magnetism of Fe/Au multilayers

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Abstract

By *ab initio* LMTO calculations in atomic-sphere approximation we have studied the interlayer exchange coupling between Fe films separated by Au spacers in infinite Fe/Au multilayers with (001) interface orientation. We also performed detailed calculations of the magnetization and charge profiles across the system. We find an enhancement of the Fe moments at the interface, which amount to $\approx 2.8\ \mu_B$ instead of the bulk value of $2.2\ \mu_B$, and we also find a slight magnetic polarization of the order of $0.01\ \mu_B$ at the Au interface layers. These results do not depend sensitively on the lattice constants assumed in the calculation. When we try to optimize our results with respect to the ratio R_{Fe}/R_{Au} of the Wigner-Seitz spheres for the mutual components, we often find the optimum near charge neutrality of the interface monolayers: However, this is not always the case, and usually the sign and the magnitude of the exchange coupling depend sensitively on the optimal choice of the above-mentioned ratio. In particular, for Fe_5/Au_3 we find an anomaly with a large dipole moment at the interface and a related anomaly of the exchange coupling.

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1 Introduction

It is well known meanwhile that in metallic magnetic multilayers with ferromagnetic films (e.g. Fe, Co,...) separated by non-magnetic or antiferromagnetic spacers (e.g. Cu, Cr,...) there exists a pronounced indirect exchange coupling between the magnetic layers, mediated by the coherent tunneling of the electrons through the spacer ([1, 2, 3]). This coupling is explained by RKKY-like or electronic Fabry-Perot-like interference theories (e.g. [4, 5]) or by theories stressing the (partial) confinement of certain kinds of the electrons (e.g. [6]) in specific layers, or by *ab initio* calculations (e.g. [7, 8, 9]). Here we have applied an *ab initio* calculation to (001)-Fe_n/Au_m multilayers, which are all periodically continued in the direction perpendicular to the layers, with the purpose to study in detail not only the above-mentioned exchange coupling, but also to monitor the changes of the magnetic moment and charge density profiles near the interface. It was also our intention to see, how the results depend on details of the computation concerning the atomic radii in an atomic-sphere approximation (ASA) for a binary system. In this respect, our results turn out to be interesting in itself, and often they do not depend sensitively on the above-mentioned details. However, there are exceptions, which we point out, and which show that sometimes the standard ab-initio calculations, where the atomic positions at the interface are fixed, are questionable in the present context, i.e. one should expect considerable interface relaxations or even reconstructions, which are accompanied by changes in the magnetic coupling *et vice versa.*

2 The formalism

We use the LMTO (Linearized Muffin-Tin Orbital) program of O.K. Anderson and coworkers in its non-relativistic version and in the atomic sphere approximation (ASA), however with the so-called 'combined corrections' and the accurate k-space summation, [10, 11]. (In all our calculations, the number of k-points was $8000 = 20\times\ 20\times\ 20$).

The 'combined corrections' take into account (i) the states of higher angular momentum, e.g. the f-states, which are otherwise neglected, as usual, in our LMTO calculations for Fe and Au, and (ii) at the

same time they take into account the fact that the ASA spheres are, on one hand, *overlapping* in parts of the space, whereas on the other hand there remain 'interstitial' regions, which are completely outside the spheres: For elemental metals the 'combined corrections' reduce the corresponding mistakes efficiently, [10, 11]; however for the present binary multilayer systems these mistakes may still belong to the main weaknesses of the ASA (see below, and [12]).

Concerning the structure, we use a hard-core model for Au grown on bcc-Fe (a=2.78 $\mathring{A}$), or sometimes, if explicitly stated, also Fe grown on fcc Au, with (001) interfaces (fcc nearest-neighbour Au-Au distance: 2.88 $\mathring{A}$). As usual, we assume that the hard-core diameters of the atoms are identical with the nearest-neigbour distances in both structures). These simplified structural models for Fe_n/Au_m multilayers seem justified by the thorough studies of Fullerton *et al.*, [13].

Our calculation is fully self-consistent concerning charge densities, spin densities, and energies (with the usual contributions from the kinetic energy, attraction of the electrons by the nuclei, Madelung energies from atoms with different nuclear charge, Coulomb repulsion and exchange-correlation energy of the electrons), see [10], and as in our preceding calculations, [7, 8, 9, 14], the standard local spin density approximation (LSDA) of van Barth and Hedin has been used, [15].

In the atomic sphere approximation for a two-component multilayer system, there is however the following freedom: The 'average sphere radius' $W = [3V/(4\pi N)]^{1/3}$ is of course fixed for a given multilayer, where N is the total number of atoms in an elementary cell, and V $(= n_1V_1 + n_2V_2)$ its volume, however the ratio

$$R_1/W = \{N/[n_1 + n_2(V_2/V_1)]\}^{1/3} \tag{1}$$

is not. Here n_1 resp. n_2 are the numbers of Fe resp. Au atoms in the elementary cell, and V_1 resp. V_2 are the corresponding atomic volumes, i.e. $V_i = 4\pi R_i^3/3$.

In our former calculations, we have always taken for V_1 and V_2 those values, which these quantities have in the elemental metals, namely $V_{Fe} = 11.82$ $\mathring{A}^3$ and $V_{Au} = 16.98$ $\mathring{A}^3$, which corresponds to $R_1/W \approx 0.94$ for $n_{Fe} = n_{Au} = 1$. Another choice would be $R_i/W = 1$. However here we consider R_1/W as a *variational parameter* for our calculation, and thus we present results below, where R/W $(=R_1/W = R_{Fe}/W)$

is varied between ≈ 0.94 and 1. We stress at this place that every variation of R_1 must of course be accompanied by a well-defined change of R_2, such that $n_1 R_1^3 + n_2 R_2^3$ remains fixed. Also all atomic positions remain fixed in our approach.

3 Results

In Fig. 1, we present results for Fe_2/Au_2-multilayers, always with the above-mentioned (001)-orientation. The figure contains four parts, namely

(i) in the upper-left quadrant the total charge Q ($= Q_{tot}$ in the figures), which is contained, according to our calculation, in a Fe ASA-sphere at the interface layer, is presented in units of the electronic charge q_e. The quantity Q thus measures the local deviation from charge neutrality at the atom considered. (Positive $Q[q_e]$ means an excess of electronic charge, compared with the neutral atom.) One can see from Fig. 1 that the interface is electrically neutral at $(R/W) \approx 0.959 \pm 0.001$, whereas for larger (smaller) ratio R/W the Fe interface layer contains a higher (smaller) amount of electronic charge, as expected. The dependence of Q on R/W is linear.

(ii) In the lower-left quadrant of Fig. 1, the minimum of the total energy per antiferromagnetic elementary cell of 8 atoms appears also at the same value $R/W \approx 0.959 \pm 0.001$, and to the accuracy of the drawing the results cannot be distinguished for mutually parallel resp. antiparallel alignment of the ferromagnetic layers.

(iii) But on the upper-right quadrant of Fig. 1 the energy difference $\Delta E := E^{\uparrow\uparrow} - E^{\uparrow\downarrow}$ per antiferromagnetic unit cell (8 atoms) is presented, and one sees that the *ferromagnetic state* is energetically slightly favoured at the above-mentioned value of $R/W \approx 0.959 \pm 0.001$, whereas for $R/W \lesssim 0.95$ and $R/W \gtrsim 0.98$ one would predict a different mutual orientation, namely the antiferromagnetic one.

(iv) Finally the lower-right quadrant of Fig. 1 shows the Fe moments at the interface, which vary only slightly between 2.7 and 2.9 μ_B, when R/W increases from 0.94 to 1, and at the 'optimal value' of $R/W \approx 0.959$ the moment is $\approx 2.775 \pm 0.005\ \mu_B$, both for mutual parallel resp. antiparallel alignment.

These results were calculated for Au grown on Fe, however similar

results are also obtained for the slightly different structure corresponding to Fe grown on Au. Since these results do hardly differ, they are not plotted here.

As a consequence, to get relevant results for the composition n=m=2 of our multilayer it *appears* that, to a first approximation, one should simply take that value of R/W, where one has charge neutrality at every atom. However, this simple recipe does apparently not work as a general rule: E.g. for $n = m = 1$ we find that the minimum of the total energy is taken for a higher value of R/W slightly below 0.98 with $Q[q_e]$ as large as ≈ 0.125, whereas charge neutrality would again happen near $R/W \approx 0.96$. Also for $n = 5$, $m = 3$ we obtain pronounced deviations from the above-mentioned 'postulate' (see below); so, to our experience, it would be unreasonable to take local charge neutrality as an unchecked 'natural apriori-approximation'.

In fact, in Fig. 2a we present our results for the Fe_5/Au_3 multilayer, again for Au grown on Fe. The minimum of the total energies per antiferromagnetic elementary cell of 16 atoms, both for mutually parallel and for mutually antiparallel orientation of the Fe magnetizations of subsequent Fe sandwiches, happens again for $R/W \approx 0.96$ in this case, but now for this value there is a large charge transfer of $Q \approx -0.05\ q_e$ at the Fe interface layers, i.e. the Fe rsp. Au layers at the interface carry a positive (resp. negative) charge of $\mp 0.05\ q_e$ per atom. In contrast, charge neutrality at the interface would now happen at a significantly higher value of $R/W \approx 0.973$. At this higher value, the exchange interaction is *antiferromagnetic* and relatively small (i.e. the energy difference ΔE, upper-right quadrant of Fig. 2a, is positive, of the order of 0.0001 Ry), whereas at the sharp minimum of the total energy in Fig. 2, i.e. at $R/W \approx 0.96$, the exchange energy is definitely ferromagnetic and one order of magnitude larger, namely $\Delta E := E^{\uparrow\uparrow} - E^{\uparrow\downarrow} \approx -0.003$ Ry for our antiferromagnetic unit cell of 16 atoms.

We have repeated these subtle calculations for a slightly modified structural model, corresponding now to Fe grown on Au, see Fig. 2b, and on this occasion we have produced data for an additional point of R/W just above the minimum at $R/W \approx 0.96$. From this additional calculation it seems that the pronounced minimum at $R/W \approx 0.96$, with $\Delta E \approx -0.003$ Ry, is even much steeper than expected from Fig.2a, and it seems that here some kind of resonance phenomenon happens

which is beyond the simplifications made in the LMTO-ASA method, see below.

In fact, if one plots the charge Q per atom for the eight different layers of our periodically continued and ferromagnetically polarized Fe_5/Au_3 system against the layer index, one gets the results presented in Fig. 3. Here the solid circles are for the energetically stable configuration with $R/W \approx 0.96$, where a strong negative dipole moment (the Fe sphere has a positive charge, since q_e is negative) at the interface from layer five (Fe) to layer 6 (Au) is observed. In contrast, for the above-mentioned configuration with $R/W \approx 0.973$, (the open circles), the interface dipole moment is reduced by two-thirds in magnitude, and is, moreover, *inverted in sign*. This kind of behaviour gives rise to speculations that this approximate multivaluedness may be resolved by some kind of interface reconstruction where the large dipole moments are reduced to quadrupole moments, or by some kind of interdiffusion, or by the formation of an interface alloy [16]: These possibilities, to be studied for systems as large as the present one, are beyond our present computational abilities. To our opinion, they demand an extremely accurate treatment by a full-potential method, i.e. beyond the ASA, beyond LDA, for more general structures, and perhaps also with non-collinear spin configurations.

Here it should of course be stressed that in Fe_5/Au_3 one has actually three non-equivalent Fe layers and two non-equivalent Au layers, so that our approach with only one variational parameters should at least in principle be replaced by an approximation with four variational parameters, $(R_{Fe})_i$, with i=1,2,3, and $\alpha := (R_{Au})_1/(R_{Au})_2$ (see the footnote [17]), which is however again beyond our computational capabilities. Instead, we restricted ourselves to the case where the first three variational parameters, $(R_{Fe})_i$, are equal and the fourth parameter, α, is 1. Our above-mentioned parameter value of $R/W \approx 0.973$, corresponding to the flat local minimum of the energy difference, might thus in fact be closer to the (four-dimensional) global energy minimum than the above-mentioned value of $R/W \approx 0.96$, where according to our (one-dimensional) variational approximation the minimum is situated.

Interestingly, the anomalies seen in Fig. 2 apparently do not show up in in other quantities: In particular, when plotting the optimal

radii R_{Fe} and R_{Au} determined in our calculation for the four systems (1) Fe_1/Au_1, (2) Fe_2/Au_1, (3) Fe_2/Au_2, and (4) Fe_5/Au_3, we find the results presented in Fig. 4. From this figure one concludes that the optimal value of R_{Fe} in our calculations practically does not change, and it is only R_{Au} that varies. If one extrapolates this result, i.e. the approximate constancy of the 'optimal' R_{Fe}, also to other compositions, it may be quite useful, since with W and R_{Fe} also the optimal values of R_{Au} would be known.

In Fig. 5 we also plot profile-functions of the magnetic moments. From the figure one can not only see that the iron moments near the interface are enhanced, as mentioned above, but one can also see that the Au atoms, too, become slightly polarized at the interface, to the order of 0.01 μ_B. This Au polarization is parallel to that of Fe, whereas at the second Au layer, it is antiparallel, but still much smaller. Experimentally such small moments can be measured by X-ray dichroism, [18], and the enhanced Fe moments at an (001) interface to Au have been found by experimental work in our department, [19].

In Fig. 6a,b and Fig. 7 we finally plot results for the interlayer exchange coupling J as a function of the Au thickness x (Fig. 6) and of the Fe thickness, (Fig. 7), for different systems. Obviously it is necessary to take the optimized value of R/W, and not the 'old' one obtained with the ratio R_{Fe}/R_{Au} taken from bulk calculations; i.e. from Fig. 6 and Fig. 7 we find that the computational results for the exchange interaction are astonishingly sensitive to the choice of R/W. One could be tempted to extrapolate the 'new' results of Fig. 6a by a decaying spatially-sinusoidal exchange oscillation of the form $\Delta E \sim 0.0006$ Ry $\times \sin[\pi \cdot (x-2)/3]/(x/3.5)^2$, i.e. with a 'period' of roughly 6 Au monolayers. This would look reasonable in view of the expected asymptotic behaviour, [4, 5]; however actually, in Fig. 6, one is still very far from the asymptotic regime; so this extrapolation should not be taken serious, although from $x = 2$ to $x = 5$ it fits the data quite well. At the same time, from Fig. 6b it seems that the 'unnatural behaviour', particularly with the drastic change observed between Fe_3Au_4 and Fe_3Au_5 with the 'old' parameters, looks much smoother now, and more reasonable, with the new optimized parameters, in agreement with the smooth behaviour already mentioned in connection with Fig. 4. Finally in Fig. 7 it is obvious that the dependence on n_{Fe} is more drastic

for the Fe_n/Au_1 system than for Fe_n/Au_2, which is reasonable, since also the deviations from local charge neutrality are much larger in the first-mentioned case:

Actually, at the optimal value of the variational parameter R/W, we have observed the most pronounced deviations from local charge neutrality for Fe_1/Au_1 multilayers, whereas for Fe_2/Au_2 we had charge neutrality at the optimum. The difference is plausible on symmetry reasons :

In the first-mentioned case, an Fe atom has two Au neighbours at the right-hand rsp. left-hand side, say, and charge transfer from these neighbours into the overlap region of the Fe ASA-sphere sums up to a non-zero value. In contrast, in the second case, an Fe-atom has one Au neighbour, say, to the left, and a Fe neighbour to the right; if there is now a charge transfer in the overlap region from Au to Fe, i.e. from the left, say, due to a *reduction* $\delta R_{Au} < 0$, this corresponds to an *enhancement* $\delta R_{Fe} > 0$ for the right neighbour. I.e. at the overlapping region to the right the charge transfer from the Fe neighbour will probably have opposite sign to that one observed at the overlapping region to the left. This will lead to largely compensating transfers, and to a correspondingly small result for $|Q|$. Therefore, even if for Fe_2/Au_2 multilayers the single ASA spheres are essentially charge-neutral, they will probably carry a large non-trivial charge-density, e.g. positive rsp. negative, near the left-hand rsp. right-hand overlap regions of the ASA spheres; whereas for Fe_1/Au_1 these regions will carry charges of the same sign leading to large values of $|Q|$. In the overlapping regions and nearby, the magnitudes of the local charge transfer should be of the same order in both cases.

4 Conclusions

We have calculated the spatial variation of the charge-density, the profile-functions of the local moments, and the exchange coupling energy between successive Fe films, for (001)-Fe_n/Au_m multilayers, by a LMTO calculation in ASA and LSDA approximations, and observed subtle behaviour: Varying the ratio of the Wigner-Seitz radii R_{Fe}/R_{Au} for given value of the 'average Wigner-Seitz radius W', see eq. (1), we found that often – but not always – the best values for the total energy

(and as a consequence also for the interlayer exchange couplings of the Fe layers across the Au spacer) is obtained near 'charge neutrality' of the interfaces. In particular for Fe_1/Au_1 multilayers and Fe_5/Au_3 multilayers this was *not* the case. For the last-mentioned system a subtle kind of 'resonant behaviour' as a function of R/W appeared near the value $R/W = 0.96$, and as a consequence there may be in this case a strong interface reconstruction, or other possibilities like an interface alloy, or noncollinear states, which is beyond the approximations and limitations of the present approach. In fact, it is our belief that with the present paper, which first originated as a case study, we have also made obvious that such subtle problems as the present one, or even more subtle problems as the just mentioned 'other possibilities', should better be treated – if possible – by a full-potential formalism, and possibly with non-collinear spin states. At the same time there is a demand for conclusive experiments.

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But in their calculation they changed the interlayer distances in accordance with the variations δR_i, whereas in our calculation all atomic positions are kept fixed. In fact, in [13] the authors observed large effects only due to the Pd atoms. In particular, in a study of Fe/Au bilayers and Fe/Pd/Au trilayers, grown by molecular epitaxy on Ag(001), it was also found in [13] that the Fe and Au layers were well represented by their bulk structure, in agreement with our structural assumptions.

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Figure captions

Fig.1: (i) The charge Q_{tot} in an interface Fe ASA sphere (always $= Q$ in the text) in units of the (negative) electronic charge q_e, (ii) the total energy E_{tot} ($= E$ in the text) of the antiferromagnetic unit cell containing eight atoms, (iii) the energy difference $\Delta E = E^{\uparrow\uparrow} - E^{\uparrow\downarrow}$, and (iv) the magnetic moment of the interface Fe ASA sphere are plotted against the ratio R/W, where R is the radius of the Fe sphere used in our LMTO-ASA calculation for Fe_2/Au_2 multilayers, while W is fixed by the equation $4\pi W^3/3 = N/V$, where V is the volume and N the number of atoms of our multilayer. The 'hard-core' structural model has been produced by growing Au on bcc-Fe, with (001)-interfaces. Our multilayers are always periodically continued in the direction perpendicular to the interfaces.

Fig.2a: The same as in Fig.1, but for Fe_5/Au_3 multilayers.

Fig.2b: The same as in Fig.2a, but for Fe grown on Au. In the lower right figure, the solid and dotted lines, respectively, remind to the slightly different results in Fig.2a. The lines are a guide to the eye only, and Fig.2b, part (iii) for ΔE, shows that actually near the resonance more points are needed.

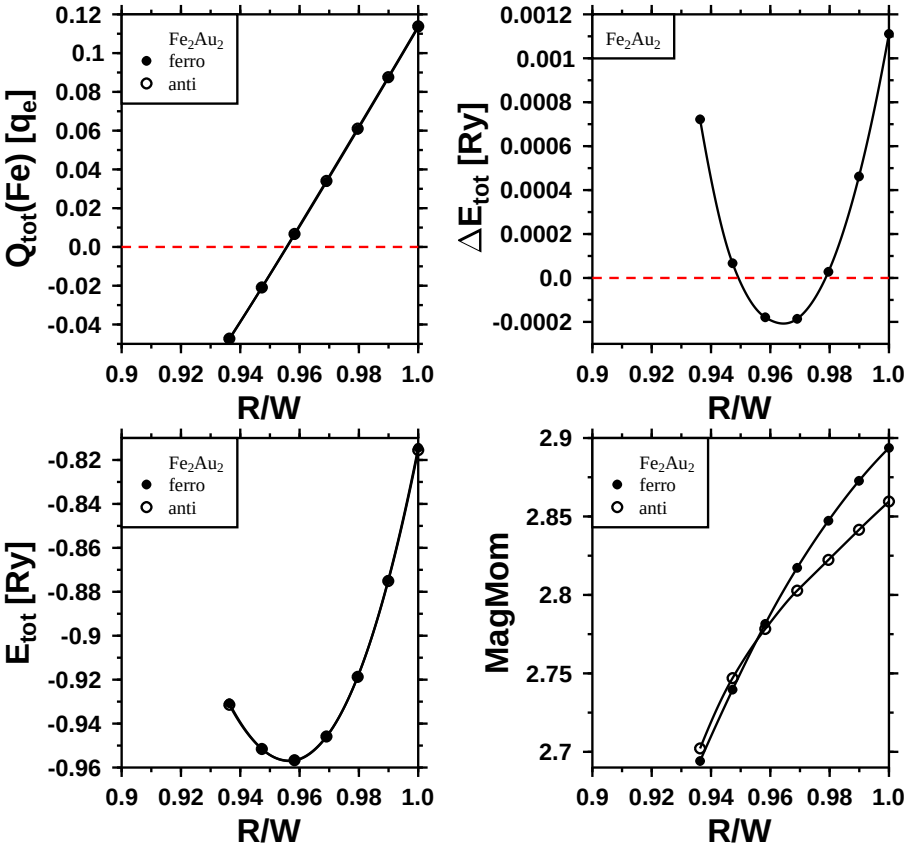
Fig.3: For the stable state at $R/W \approx 0.96$ in Fig.2a (full circles), and for the different state at $R/W \approx 0.975$ (open circles), the charge Q_{tot} contained in the respective atomic spheres is plotted against the layer index. Layers 1, ..., 5 correspond to Fe, the rest to Au. Note the drastic change of sign and magnitude at the layers 5 and 6.

Fig.4: For the cases $1\hat{=}Fe_1/Au_1$, $2\hat{=}Fe_2/Au_1$, $3\hat{=}Fe_2/Au_2$, and $4\hat{=}Fe_5/Au_3$, the radius R_{min} corresponding to the absolute minimum of E_{tot} (see e.g. Figs.1–2 for cases 3 and 4) is plotted for Fe (filled circles) and Au (open circles).

Fig.5: The profiles of the magnetic moments per ASA sphere across the multilayer are plotted against the layer index for Fe_2/Au_3, Fe_3/Au_5, Fe_5/Au_1 and Fe_5/Au_2, both for parallel and antiparallel mutual spin orientation of the Fe sandwiches. The induced Au moments have been enlarged by a factor of 10.

Fig.6a: The energy difference $\Delta E = E^{\uparrow\uparrow} - E^{\uparrow\downarrow}$ per antiferromagnetic elementary cell is plotted against the number x of Au layers for Fe_2Au_x multilayers. The filled circles are the new results with the optimized ratio of R/W, whereas the open circles correspond to the ratio R/W

obtained from the bulk values of R_{Fe} and R_{Au}.
Fig.6b: The same as Fig.6a, but for Fe_3/Au_x multilayers.
Fig.7: The same as in Fig.6, but now in both cases the 'new method' is used and the Fe thickness is varied. The 'filled circles' are for Fe_x/Au_1, the 'open circles' for Fe_x/Au_2.



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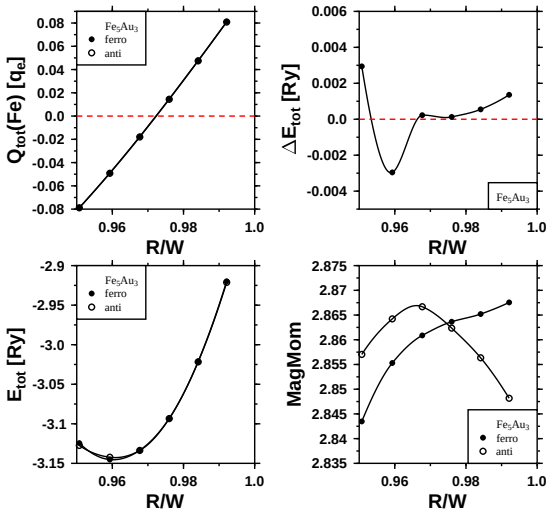

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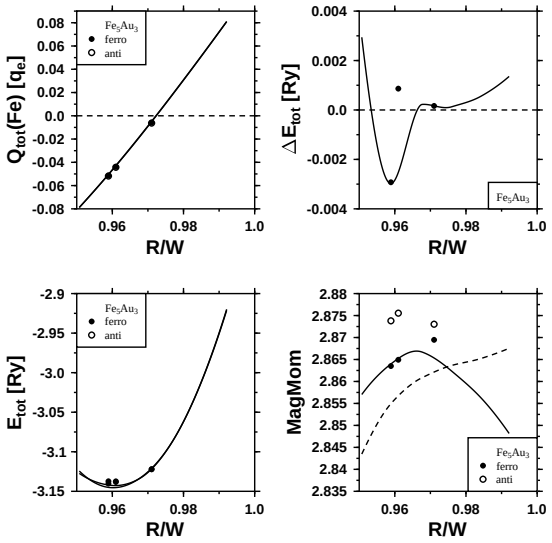

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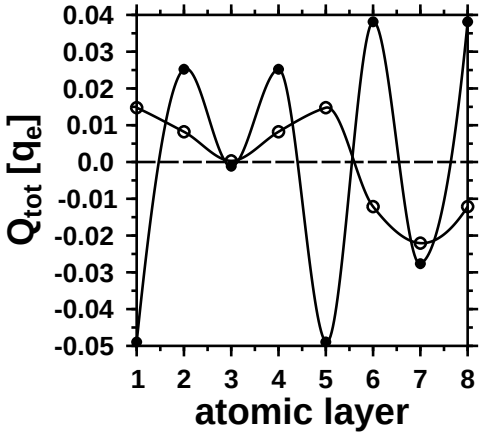

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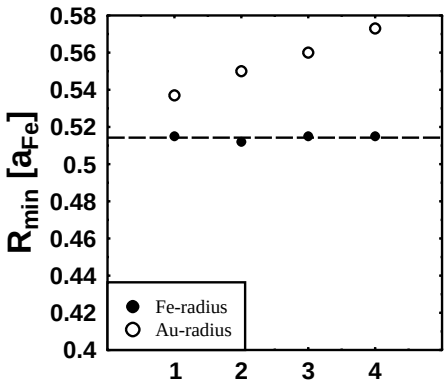


Fig.4: For the cases $1\hat{=}Fe_1/Au_1$, $2\hat{=}Fe_2/Au_1$, $3\hat{=}Fe_2/Au_2$, and $4\hat{=}Fe_5/Au_3$, the radius R_{min} corresponding to the absolute minimum of E_{tot} (see e.g. Figs.1–2 for cases 3 and 4) is plotted for Fe (filled circles) and Au (open circles).

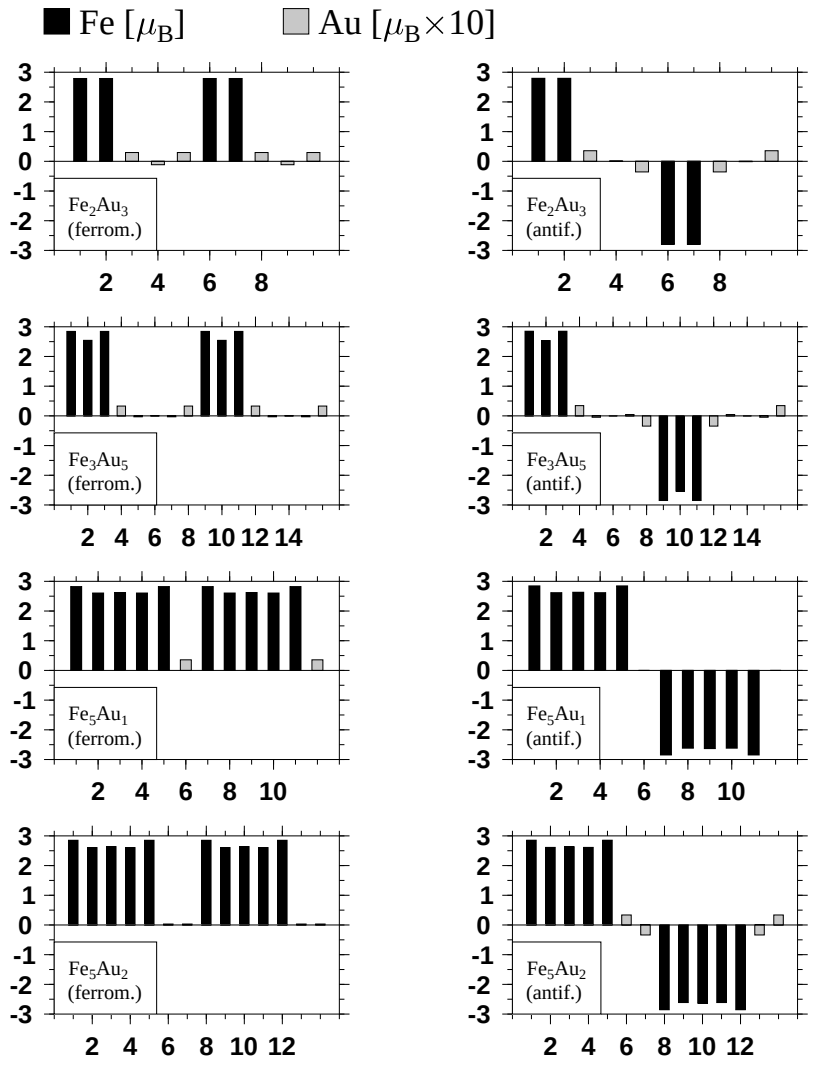
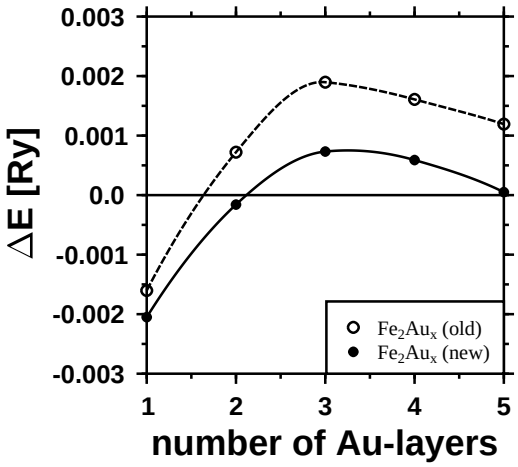
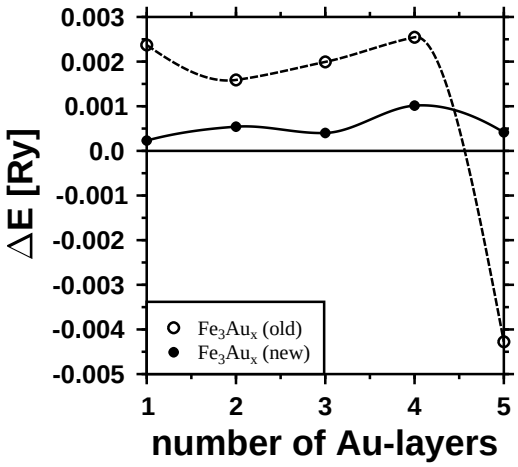


Fig.5: The profiles of the magnetic moments per ASA sphere across the multilayer are plotted against the layer index for Fe_2/Au_3, Fe_3/Au_5, Fe_5/Au_1 and Fe_5/Au_2, both for parallel and antiparallel mutual spin orientation of the Fe sandwiches. The induced Au moments have been enlarged by a factor of 10.



Fe_2Au_x

Fig.6a: The energy difference $\Delta E = E^{\uparrow\uparrow} - E^{\uparrow\downarrow}$ per antiferromagnetic elementary cell is plotted against the number x of Au layers for Fe_2/Au_x multilayers. The filled circles are the new results with the optimized ratio of R/W, whereas the open circles correspond to the ratio R/W obtained from the bulk values of R_{Fe} and R_{Au}.



Fe_3Au_x

Fig.6b: The same as Fig.6a, but for Fe_3/Au_x multilayers.

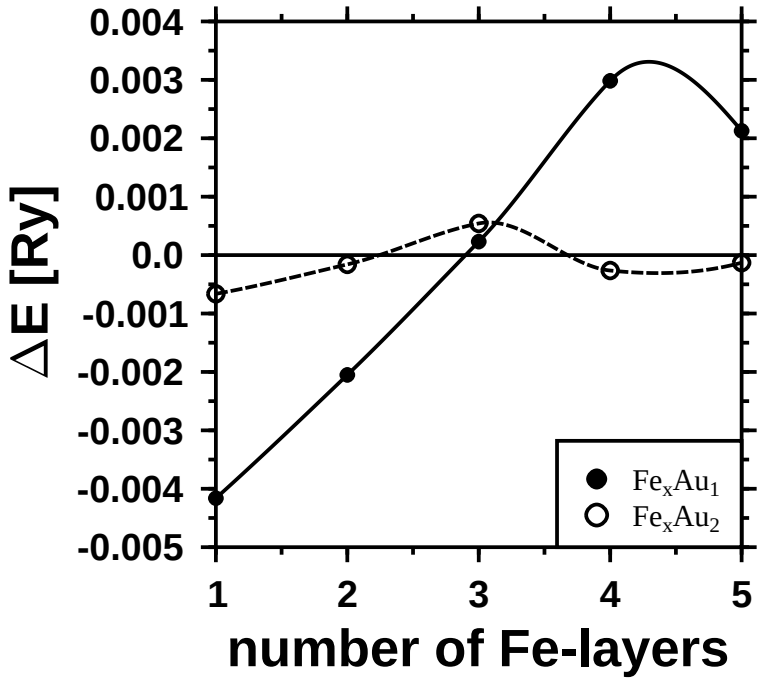


Fig.7: The same as in Fig.6, but now in both cases the 'new method' is used and the Fe thickness is varied. The 'filled circles' are for Fe_x/Au_1, the 'open circles' for Fe_x/Au_2.